Suppression of superconductivity in the Hubbard model by buckling and breathing phonons

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We study the effect of buckling and breathing phonons, relevant for cuprate superconductors, on the d-wave superconductivity in the two-dimensional Hubbard model by employing dynamical cluster Monte Carlo calculations. The interplay of electronic correlations and the electron-phonon interaction produces two competing effects, an enhancement of the effective d-wave pairing interaction, which favors d-wave superconductivity, and a strong renormalization of the single-particle propagator, which suppress superconductivity. Due to the later effect we find that buckling and breathing phonons suppress the superconductivity in the region of parameter space relevant for cuprate superconductors.

Introduction. Many experiments, including Raman [1], neutron scattering [2], and photoemission [3, 4] find clear evidence of electron-phonon (EP) interaction in high T_c materials. While it is widely accepted that strong electronic correlations play a fundamental role in the mechanism of high temperature superconductivity, the role of EP interaction is under hot debate.

The phonons believed to be the most relevant to the cuprates are the buckling (BC) and the breathing (BR) modes [1, 2, 3, 5, 6, 7], defined, respectively, by the out-of-plane and in-plane displacement of the oxygen ions. Previous investigations suggest that the symmetry of these phonon modes is significant. There are arguments suggesting that coupling to the out-of-plane oxygen BC or the local Holstein (H) phonons, enhance the d-wave pairing interaction [8, 9, 10, 11, 12], whereas, the BR mode has been found to suppress the interaction [9, 10, 11]. It also was shown that the electronic correlations in the presence of EP coupling strongly enhance polaron formation [13, 14, 15] and renormalize the quasiparticle (QP) weight, an effect which suppresses superconductivity.

In this letter we employ the dynamical cluster approximation (DCA) [16, 17] to study two models relevant for cuprates, the Hubbard model with BC and BR phonons. We also extend the work on superconductivity in the Hubbard-Holstein model [15]. DCA has proved to be one of the few techniques able to capture the superconducting properties of strongly correlated systems [17]. We investigate the role of phonons on superconductivity in the region of small and intermediate doping where the antiferromagnetic (AF) correlations are strong. In agreement with previous investigations, we find enhancement of the d-wave pairing interaction by H [8, 15] and BC [9, 10, 11, 12] phonons. Moreover we find an enhancement of the d-wave pairing interaction even for BR phonons contrary to some predictions [9, 10, 11]. However, despite the enhancement of the d-wave pairing, we find a suppression of the superconducting T_c for all three modes, due to the strong renormalization of the electronic single-particle propagator.

Formalism. The Hamiltonian for each model, Hubbard-Holstein (HH), Hubbard-Buckling (HBC) and Hubbard-Breathing (HBR), can be written as

$$H = H_U + H_{ph} + H_{ep} \tag{1}$$

where

$$H_U = -t \sum_{\langle ij\rangle\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} \tag{2}$$

is the Hubbard part with nearest-neighbor hopping t and on-site repulsion U. For H phonons, described as a set of independent oscillators at every site i which couple locally to the electronic density,

$$H^H_{ph} + H^H_{ep} = \sum_i \frac{p_i^2}{2M} + \frac{1}{2} M\omega_0^2 u_i^2 + g n_i u_i, \tag{3}$$

where $\{u_i, p_i\}$ are canonical conjugate coordinates for each oscillator with characteristic frequency ω_0. The BC (BR) phonons are independent out-of-plane (in-plane) oscillators on each bond $i + \hat{\gamma}/2$, with $\hat{\gamma} = \hat{x}, \hat{y}$, such that

$$H^{BC,BR}_{ph} + H^{BC,BR}_{ep} = \tag{4}$$

$$= \sum_{i,\gamma} \frac{p^2_{i+\hat{\gamma}/2}}{2M} + \frac{1}{2} M\omega_0^2 u^2_{i+\hat{\gamma}/2} + g(n_i \pm n_{i+\hat{\gamma}}) u_{i+\hat{\gamma}/2}$$

where the last term of Eq. 4 with plus (minus) describes the coupling to the BC (BR) phonons. The dimensionless EP coupling, defined as the ratio of the single-electron lattice deformation energy to half of the electronic bandwidth $W/2 = 4t$, is $\lambda^H = 2g^2/(2M\omega_0^2 W)$ and $\lambda^{BC,BR} = 4 \times 2g^2/(2M\omega_0^2 W)$ [24], with an extra factor of four in $\lambda^{BC,BR}$ due to local coordination. Note that in

general the coupling to the BC mode implies both modulation of orbital energy and hopping integrals [7]. However, due to the technical difficulties associated with off diagonal EP coupling, we consider here only the former effect as was done previously in Ref. [9, 10].

To study the Hamiltonian (1) we employ the DCA, a cluster mean-field theory which for a two dimensional system maps the original lattice model onto a periodic cluster of size $N_c = L_c^2$ embedded in a self-consistent host. Correlations up to a range L_c are treated explicitly, while those at longer length scales are described at the mean-field level. With increasing cluster size, the DCA systematically interpolates between the single-site dynamical mean field result and the exact result, while remaining in the thermodynamic limit. Cluster mean field calculations on the simple Hubbard model successfully reproduce many of the features of the cuprates, including a Mott gap and strong AF correlations, d-wave superconductivity and pseudogap behavior [17].

We solve the cluster problem using a quantum Monte Carlo (QMC) algorithm [20] modified to perform the sum over both the discrete field used to decouple the Hubbard repulsion, as well as the phonon field u. The space of configurations of the latter field is significantly larger than the former. In part, this is offset by the strong correlations of the phonon field in Matsubara time. Therefore, in the QMC Markov process, correlated changes, in which adjacent phonon fields in time are moved together, are mixed in with local moves to reduce the autocorrelation time. Nevertheless, the present code including the effect of phonons requires significantly more CPU time than required for the Hubbard model. Thus, most of the present calculations are restricted to clusters of size $N_c = 4$. Nevertheless we check the robustness of our conclusions by employing calculations on larger clusters of size $N_c = 16$.

Results. In a previous paper, addressing the HH model [15], we show that the synergistic interplay of AF correlations and the EP interaction strongly enhances both polaron formation and antiferromagnetism. Since the effective EP coupling is inversely proportional to the kinetic energy of the holes, the AF correlations, which reduce the mobility of the holes, enhance the effective EP coupling. On the other hand, since at finite doping the antiferromagnetism is suppressed by the hole motion, the decrease in hole mobility due to EP coupling increases the antiferromagnetism. Considering the BC and the BR phonons we find a similar behavior indicative of enhanced polaron formation. In Fig. 1 -a we show that the AF susceptibility at 5% doping is strongly enhanced by coupling with any of the three phonon modes. The EP coupling also reduces the Matsubara QP weight, $Z_0(T) = 1/(1 - \mathrm{Im}\Sigma(K, i\pi T)/\pi T)$ (Fig. 1 -b for momentum $K = (0, \pi)$), and increases the kinetic energy (Fig. 1 -c) [25]. For all three models the local moment, $\mu^2 = \langle (n_\uparrow - n_\downarrow)^2 \rangle$, at low temperature has a large value, close to that corresponding to the $\lambda = 0$ case (Fig. 1

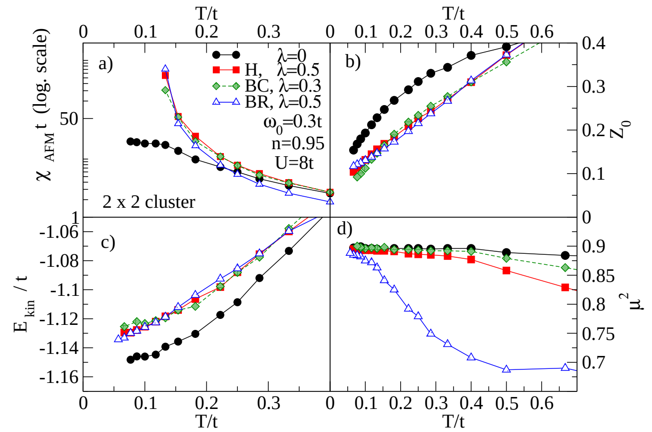

FIG. 1: (color online) a) AF susceptibility χ_{AF}, b) Matsubara QP fraction $Z_0 = 1/(1 - \mathrm{Im}\Sigma(K, \pi T)/\pi T)$ at $K = (0, \pi)$, c) kinetic energy $E_{kin} = \sum_{k\sigma} \epsilon(k) n_{k,\sigma}$ and d) local moment $\mu^2 = \langle (n_\uparrow - n_\downarrow)^2 \rangle$ versus T for HH, HBC and HBR models at 5% doping. All three modes show enhanced polaron formation at low T.

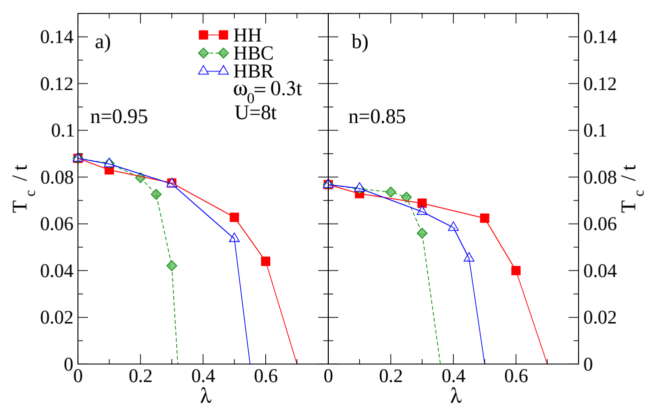

FIG. 2: (color online) T_c versus λ for HH, HBC and HBR models at (a) 5% and (b) 15% doping for $\omega_0 = 0.3t$, $U = 8t$ and $N_c = 4$.

-d), due to reduction of the effective hole hopping. However, aside from the similarities between the three models, there are also significant differences. We find that for the HBC model the same value of EP coupling produce much stronger effects then for the HH and HBR models. For example at 5% doping a value of $\lambda^{BC} = 0.3$ produces effects similar to $\lambda^{H,BR} = 0.5$. The temperature dependence of the local moment (Fig. 1 -d) as well as of other quantities such as DOS (not shown) is much stronger in the HBR model.

In Fig. 2 we show the dependence of superconducting T_c versus EP coupling for the three models for $\omega_0 = 0.3t$ at 5% and 15% doping. We find T_c decreases with increasing λ, weakly for small λ and then quite abruptly for $\lambda > \lambda_c$. We find that $\lambda_c^{H,BC,BR} \approx 0.5, 0.25, 0.4$ [26]. Notice that the decrease of T_c with λ for HBC model is

much sharper once $\lambda > \lambda_c^{BC}$.

Previous investigations predict an enhancement of the phonon contribution to the d-wave pairing interaction when the coupling with BC or H phonons is considered [8, 9]. However, an increase of the interaction which favors d-wave pairing does not necessarily imply an increase of T_c, since the reduction of the QP weight and DOS at the Fermi level, $N(0)$, has the opposite effect. We find for all three models an increase of the d-wave pairing interaction. However, in spite of this, the T_c is reduced as shown in Fig. 2. To understand this dichotomy, we must disentangle the effects of the pairing interaction from renormalization of the single-particle propagator.

A divergent pairing susceptibility indicates the superconducting transition and hence T_c. At this instability the leading eigenvalue of the pairing matrix becomes 1. The pairing matrix $M = \Gamma\chi_0$ enters in the Bethe-Salpeter equation of the two-particle Green's function,

$$\chi = \chi_0 + \chi_0\Gamma\chi = \chi_0 + \chi_0(1-M)^{-1}M \ . \tag{5}$$

where $\chi_0 = G * G$ (the bubble diagram) describes propagation of the two particles without mutual interaction, a product of the fully renormalized single-particle propagators $G(k, i\omega) = (i\omega - \epsilon(k) + \mu - \Sigma(i\omega, k))^{-1}$. $\Gamma_{Q=0,i\nu=0}(K, i\omega; K', i\omega')$ is the irreducible interaction vertex in the particle-particle channel and can be regarded as the effective renormalized interaction. We find that for all three models the leading eigenvector $\Phi_d(K, i\omega)$ of the pairing matrix M has d-wave symmetry.

The phonons affect the pairing matrix by modifying both the effective interaction Γ and the single particle propagator G, or implicitly χ_0. To separate these effects we compare, in Fig.3, the eigenvalues of two different pairing matrices: M and M_0. M was defined above and we define $M_0 = \Gamma\chi_{00}$ with $\chi_{00} = G^0 * G^0$. $G^0(k, i\omega) = (i\omega - \epsilon(k) + \mu_U - \Sigma_U(i\omega, k))^{-1}$ is a single-particle propagator which does not account for the renormalization resulting from the EP interaction, i.e μ_U and Σ_U are the obtained by setting $\lambda = 0$. Note that the effective interaction Γ in M_0 is, however, fully renormalized by phonons.

The leading eigenvalue of M increases with decreasing T and reaches a value of 1 at the transition temperature T_c. This transition occurs at lower temperature when λ is finite, thus indicating a reduction in T_c in accordance with the phase diagram shown in Fig. 2. However, the d-wave eigenvalue of the matrix M_0 increases much faster and reaches 1 at a temperature much larger than without phonons. Since the matrix M_0 contains the fully renormalized interaction and the single-particle propagators which are not renormalized by phonons, this shows that the EP coupling strongly enhances the d-wave pairing interaction. However, the competing effect, renormalization of χ_0, is also very strong such that the net effect is a reduction of T_c.

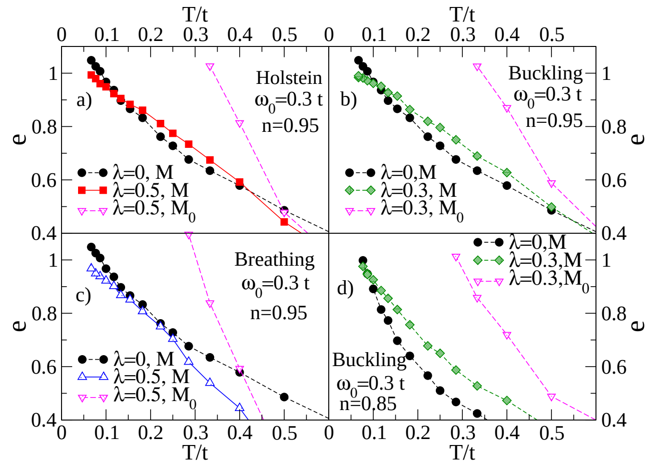

FIG. 3: (color online) d-wave eigenvalue of pairing matrices $M = \Gamma\ \chi_0$ and $M_0 = \Gamma\ \chi_{00}$ versus T on $N_c = 4$ cluster for HH (a), HBC (b) and HBR (c) models at 5% doping and HBC (d) at 15% doping. Despite the overall reduction of T_c shown by the eigenvalues of M the eigenvalues of M_0 increase strongly with decreasing T, showing that EP coupling enhances the effective pairing interaction.

Alternatively, to investigate the pairing interaction one can look at quantities such as $V_d = \sum_{K,i\omega;K',i\omega'} \Phi_d(K, i\omega)\Gamma(K, i\omega; K', i\omega')\Phi_d(K', i\omega')$ and $P_{d0} = \sum_{K,i\omega} \Phi_d^2(K, i\omega)\chi_0(K, i\omega)$ which are the respective projections of the interaction vertex and χ_0 on the subspace spanned by the d-wave eigenvector. These were previously defined in Ref. [22]. Fig. 4 -a and -b show that EP coupling enhances the effective pairing interaction V_d and strongly reduces P_{d0}, reinforcing the conclusions previously drawn from Fig. 3.

Note that we see an enhancement of d-wave pairing interaction for all three phonon modes, including BR. DCA calculations in the Hubbard model without phonons show that the main contribution to the d-wave pairing is contained in the particle-hole spin $S = 1$ channel at $Q = (\pi, \pi)$ [21], i.e. the pairing is a result of exchanging AF spin fluctuations. We speculate that the increase of the pairing interaction when EP is present results from the enhancement of the AF susceptibility. However a decomposition of the pairing vertex Γ in the fully irreducible and partially reducible particle-hole spin and density components, similar to the one done in Ref. [21] for the Hubbard model, is necessary to better understand the effect of phonons on the pairing interaction.

It is important to ask whether these results will change for other regions of parameter space relevant for cuprates or when larger clusters are considered. We find that EP coupling always reduces T_c for small phonon frequency $\omega_0 < t$. We exemplify this by showing in Fig.4 -c, -d and -e the inverse of the d-wave pairing susceptibility χ_d for some particular cases. Larger cluster, $N_c = 16$ sites, and

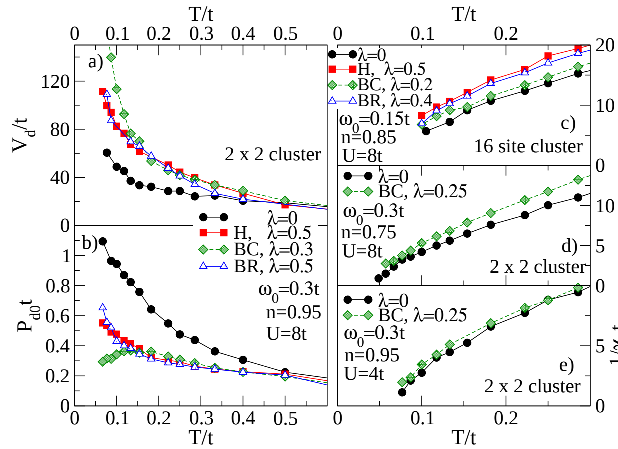

FIG. 4: (color online) a) d-wave pairing interaction V_d and b) d-wave projected bare bubble P_{d0} versus T for $U = 8t$, 5% doping, $\omega_0 = 0.3t$ and $N_c = 4$ cluster. V_d (P_{d0}) is enhanced (reduced) by EP coupling. c) Inverse of the d-wave pairing susceptibility $1/\chi_d$ for HH, HBC and HBR models for $U = 8t$, $N_c = 16$ cluster and $\omega_0 = 0.15t$ at 15% doping. d) $1/\chi_d$ for HBC model for $U = 8t$, $\omega_0 = 0.3t$, $N_c = 4$ cluster at 25% doping. e) $1/\chi_d$ for HBC model for $U = 4t$, $\omega_0 = 0.3t$, $N_c = 4$ cluster at 5% doping. We find that a finite λ always suppresses T_c.

smaller phonon frequency, $\omega_0 = 0.15t$, results are illustrated in Fig.4 -c for all three models. Even though we were unable to reach temperatures equal to T_c, due to the sign problem present in large clusters calculations, it is obvious that a finite λ suppresses the pairing susceptibility. Regarding the phonon frequency dependence of T_c, we find that, in general, T_c decreases with decreasing ω_0 (not shown), i.e. a positive isotope effect. However the magnitude of the isotope effect depends strongly on the mode, λ and doping. A detailed investigation will be presented in a subsequent publication. In Fig. 4 -d and -e we show that EP coupling reduces T_c for the HBC model in the overdoped region, 25% doping, and in the weak coupling regime, $U = 4t$. The same conclusion can be drawn for the HH and HBR models (not shown).

Our results indicate that the coupling of the electronic density to local phonons is, in general, not favorable for superconductivity in the cuprates. This result is contrary to some previous speculation [4, 23] about the role played by the EP interaction in high Tc, and therefore significant to the experimental community. Synthesis aimed at increasing T_c by designing new materials with strong EP coupling may lead to the antithetical result. A proper treatment of quasiparticle dressing is key to understanding the role played by the EP interaction. Methods that fail to properly address this point, e.g. by truncating the phonon Hilbert space, may lead to incorrect or erroneous conclusions.

Conclusions. By employing DCA with a QMC algorithm we investigate the Hubbard model with H, BC and BR phonons. We find that the interplay of EP interaction and electronic correlations in HBC and HBR models leads to synergistic enhancement of both polaron formation and AF correlations, similar to previous findings for the HH model [15]. Regarding superconductivity, all three modes produce two competing effects: a strong renormalization of the single-particle electronic propagator which suppresses superconductivity and an enhancement of the effective pairing interaction which favors d-wave superconductivity. In the region of parameter space relevant for cuprates, we find that the combination of these two effects leads to a reduction in superconducting T_c.

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[1] M. Opel *et al.*, Phys. Rev. B **60**, 9836 (1999).
[2] D. Reznik *et al.*, Phys. Rev. Lett. **75**, 2396 (1995); R. J. McQueeney *et al.*, Phys. Rev. Lett. **82**, 628 (1999).
[3] A. Lanzara *et al.*, Nature (London) **412**, 510 (2001).
[4] G.-H. Gweon *et al.*, Nature (London) **430**, 187 (2004).
[5] O. Rosch, *et al.* Phys. Rev. Lett. **92**, 146403 (2004)
[6] T. Cuk, *et al.* Phys. Rev. Lett. **93**, 117003 (2004).
[7] O. Jepsen et al., J. Phys. Chem. Solids **59**, 1718 (1998)
[8] Z.B. Huang, *et al.* Phys. Rev. B **68**, 220507(R) (2003).
[9] N. Bulut and D.J. Scalapino, Phys. Rev. B **54**, 14971 (1996).
[10] T. Sakai, *et al.* Phys. Rev. B **55**, 8445 (1997).
[11] P. Piekarz, *et al.* Phys. Rev. B **59**, 14697 (1999).
[12] C. Honerkamp, H.C. Fu, and D.-H. Lee, preprint,cond-mat/0605161.
[13] J. Zhong and H.-B. Schüttler, Phys. Rev. Lett. **69**, 1600 (1992).
[14] Peter Prelovsek *et al.* Phys. Rev. Lett. **96**, 086402 (2006).
[15] A. Macridin *et al.*, Phys. Rev. Lett. **97**, 056402 (2006)
[16] M. H. Hettler *et al.* Phys. Rev. B **58**, R7475 (1998); M. H. Hettler *et al.* Phys. Rev. B **61**,12739 (2000).
[17] Th. Maier *et al.*, Rev. Mod. Phys. **77**, 1027 (2005).
[18] O. Rösch *et al.* Phys. Rev. Lett. **95**, 227002 (2005).
[19] C. Slezak *et al.* Phys. Rev. B **73**, 205122 (2006)
[20] M. Jarrell *et al.*, Phys.Rev. **B 64**,195130 (2001).
[21] Th. Maier *et al.*, Phys. Rev. Lett. **96**, 047005 (2006).
[22] Th. Maier *et al.*, preprint, cond-mat/0606003.

[23] M. Capone *et al.*, Science, **296**, 2364, (2002).
[24] This definition of λ, common in polaron studies and used also in Ref. [18] for cuprates, does not always coincide with the Migdal-Eliashberg definition [19].
[25] The reduction of $N(0)$ and the strong increase in the static and the dynamic charge susceptibility provide additional evidence of polaron formation [15].
[26] λ_c here should not be understood necessarily as the critical EP coupling which indicates the transition to the polaron regime.